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Structure of large-angle Twist-Grain-Boundary of Chiral Liquid Crystals

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Abstract. フラストレートした液晶は位相欠陥によって数百 nm スケールの超構造を形成することがある。我々は、液晶の層状秩序と螺旋秩序のフラストレーションによる欠陥構造 (Twist-Grain-Boundary 相) の安定メカニズムを探るために、連続体 (Landau-de Gennes) モデルを数値最小化して位相欠陥の構造を解析した。特に、解析計算が困難な大きくねじれたときの構造に着目し、近似的なモデル (極小曲面) と比較した。その結果、ねじれ角の増加に伴い、液晶の分子密度と分子配向の自由度の分離により層の曲げ弾性が著しく弱化することが明らかになった。

Chiral liquid crystals exhibit a wide variety of frustrated phases. Frustration of the smectic layer order and helical orientational order causes the Twist-Grain-Boundary (TGB) phase, which consists of smectic slabs (grains) separated by planes containing arrays of screw dislocations [1] (Fig.1). Detailed understanding of this one-dimensionally twisted structure is a key to understand more complex chiral phases, such as the chiral line and the smectic blue. Theoretically, the TGB layer structure is well approximated by Scherk's minimal surface for small twist angles [3]. Here we study the frustration mechanism at larger twist angles, focusing on the local structure of a single grain boundary [4]. Such a highly deformed structure is still stable as confirmed experimentally [5].

Our method is direct numerical minimization of the Landau-de Gennes free energy, which consists of the following terms.

$$F_{D.W.} = \int dr \frac{g}{4}\left(\frac{\tau}{g}+|\Psi|^2\right)^2, \tag{1}$$

$$F_{int} = \int dr \frac{B}{2}|(\nabla - iq_0\mathbf{n})\Psi|^2, \tag{2}$$

$$F_{Frank} = \int dr \left\{\frac{K_1}{2}(\nabla\cdot\mathbf{n})^2 + \frac{K_2}{2}(\mathbf{n}\cdot\nabla\times\mathbf{n}-k_0)^2 + \frac{K_3}{2}(\mathbf{n}\times\nabla\times\mathbf{n})^2\right\}. \tag{3}$$

Here Ψ is the complex order parameter and $\mathbf{n}$ the director, with the layer compression modulus B and the Frank elastic constants K_i. We simulated one grain boundary with two adjacent smectic slabs, which are twisted by an angle α from each other. In this geometry we can exploit the 2D crystalline symmetry of the two slabs and utilize the periodic boundary condition in the plane perpendicular to the twist axis. The box boundaries in the direction along the twist axis are connected by reflection so that the two smectic slabs are tilted by $\pm\alpha/2$ from the horizontal plane. The chirality k_0 is obtained as a function of α as we minimize the free energy.

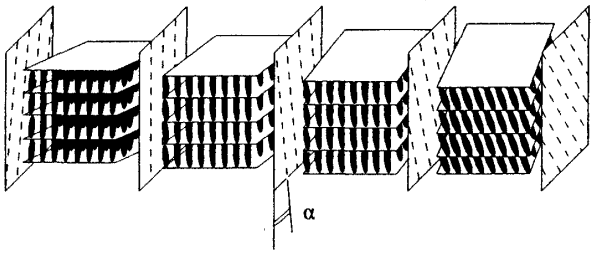

FIGURE 1. Schematic representation of the TGB structure on liquid crystals. Finite length smectic slabs are connected with an angle α by grain boundaries, where sets of parallel screw dislocations are formed.

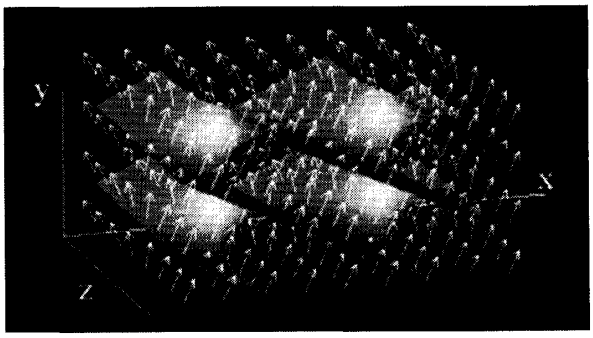

FIGURE 2. Snapshot of the TGB layer structure at $\alpha = 50°$. Shown are the isosurface $\mathrm{Re}(\Psi) = 0$ and the director in arrows.

The resultant layer structures (see Fig.2) are compared with Scherk's minimal surface. The deviation from the minimal surface is measured by squared mean curvature of the layers averaged over the sample. The deviation grows faster than linearly as a function of the twist angle. This significant deviation is found to originate from an

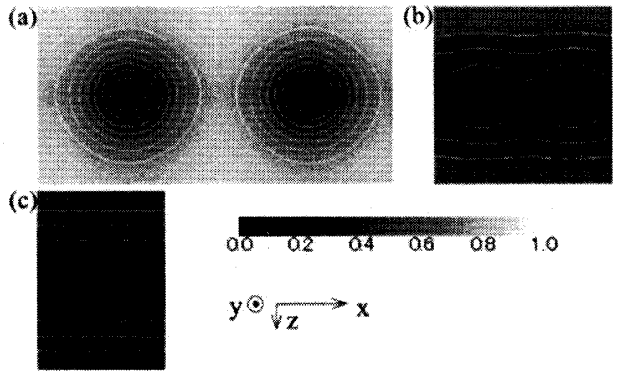

FIGURE 3. Plots of the density modulation $|\Psi|^2$ for the twist angle α = (a) 30°, (b) 60° and (c) 90° near the TGB-cholesteric transition. At higher twist angles, the smectic order melts in the whole grain boundaries.

unlocking of the layer normal from the director. To see this, we decompose the coupling energy F_{int} as follows.

$$F_{int} = \frac{B}{2}\int dr \Big| i\nabla|\Psi| - |\Psi||\nabla\phi|(\mathbf{m}-\mathbf{n}) - |\Psi|(|\nabla\phi| - q_0)\mathbf{n}\Big|^2, \quad (4)$$

Here ϕ is the phase of Ψ and $\mathbf{m} = \nabla\phi/|\nabla\phi|$ is the layer normal. As the twist angle grows, the locking term (second term) is dominated by the layer compression term (third term). As a result, the average angle between $\mathbf{m}$ and $\mathbf{n}$ approached as much as 20° at $\alpha = 90°$. This unlocking weakens the effective layer bending elasticity and causes a large mean curvature. We also studied the temperature dependence. At high temperature close to the TGB-cholesteric transition and for large twist angles, the smectic order melts in the whole grain boundary, not only near the dislocation cores (Fig.3).

In summary, we numerically minimize the Landau-de Gennes free energy of chiral liquid crystals to investigate the frustration between the smectic and helical orders, and compare the obtained layer structure with a minimal model surface. As a result, the layer bending elasticity is greatly weakened due to the unlocking of the layer orientation and the director. We further confirm a layer melting in the whole grain boundary at higher temperature and large twist angle.

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